*Heterocyclic Letters*
*Vol. 15| No.3|585-591|May-July|2025*
*ISSN : (print) 2231–3087 / (online) 2230-9632*
*CODEN: HLEEAI*
*http://heteroletters.org*

# POTENTIAL OF *ALOE VERA* MEDIATED SILVER NANOPARTICLES IN THE SYNTHESIS OF PYRIMIDINE DERIVATIVE AND INVESTIGATING THE GREEN CHEMISTRY METRICS

**Jai Shri Kaur, Preeti Singh ***

*Department of Chemistry, Faculty of Science, Swami Vivekanand Subharti University, Meerut 250005, U.P. India. Email:* sdrpreeti401@gmail.com

## Abstract
Nano biotechnology which is associated with green chemistry, exhibit great potential in the development of materials that can offer remarkable benefits to industries, human health, and environment. Among them, the nanoparticles of silver are considered to be the most studied nanomaterials due to their low chemical reactivity and higher stability. In present study, a rapid, simple, cost effective and eco - friendly methodology for the synthesis of pyrimidine derivative utilizing *Aloe vera* mediated silver cobalt nano composites has been employed. Moreover, in order to check the efficiency of methodology, green chemistry metrics was also investigated. The value of green chemistry metrics was obtained as E- factor (0.5%), process mass intensity (PMI) value (1.5%), reaction mass efficiency (RME) value (62%), and carbon efficiency (CE) value (84%). The properties of nanocatalyst make the current protocol advantageous and can be applicable to industrial level.

## Introduction
A rapid growth in the field of science and technology has led to significant increase in living standards as well as economic development. However, such types of economic developments are responsible for the remarkable degradation of environment that can be displayed by more pronounced climate changes. This scenario requires the search of a better solution in order to balance the use of environmental conservation, natural resources, and economic growth. As a result of these consequences, during the last two decades, the awareness towards the prerequisite of environment protection has been raised, hence, the great interest has been attracted towards the greener and viable technologies. Based on the Rio Declaration on Environment and Development (1992) proclaims the first principle that states “Human beings are at the center of concern for sustainable development. They are entitled to a healthy and productive life in harmony with nature”. [i] This highlighted the common challenges to decide the objectives for sustainable development and also to provide technological and scientific approaches to obtain these objectives. Though, the present scenario signifies that the present environmental quality is degrading to an anxious level which highly influences the human lives.[ii] The environmental pollution refers to the serious environment status where the concentration of organic pollutants is much higher than that of normal level

because of the presence of natural and artificial contamination.[iii] Because of the worsening situation of water, air and soil pollution the global population is suffering from unprecedented health risks.[iv-vi] For example, airborne fine particulates increases the risk of chronic and acute respiratory diseases, stroke, heart disease and also lung cancer. Similarly, water pollution leads to diarrhea-related deaths in children under the age of 5 every year.[vii] The soil pollution leads to serious health threats because of the exposure of some persistent organic pollutants.[viii] Therefore, environmental pollution, which is a hidden culprit required more concern in unraveling the etiology of obstinate health diseases. [ix-xi]. Apart from these hazards, the environment chemical hazards which are caused by organic and inorganic pollutants are gradually recognized worldwide. [xii] For instance, over the decades, most of the chemicals have been artificially prepared and then released in the environment.[xiii, xiv] Therefore, along the development of science and technology, new environmental insults which produces from the pollution of organic pollutants, heavy metals, E-waste and synthetic chemicals are emerging. [xv]

In this context, in order to protect the environment from toxic and hazardous chemicals, the new laws and regulations have been focused.[xvi, xvii] There has been a remarkable growth in the field of green chemistry both in developing the greener nanocatalysts as well adopting the greener conditions during catalysis of biologically important organic reactions.[xviii] Therefore, the chemical community by adopting the properties of green chemistry is geared up towards the designing and developing of newer compounds which are comparably less dangerous to the environment and human health.[xix] Figure 1 represents some of the important applications of green chemistry principles.

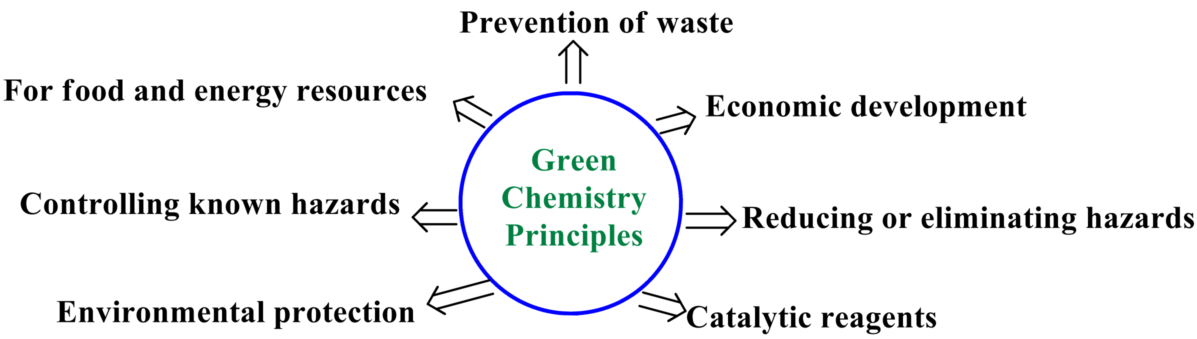



**Figure 1: Several applications of green chemistry**

Nanoparticles are considered as the building blocks of various nanotechnology applications, which commonly exhibit remarkable properties such as unique size dependent chemical and physical properties. [xx] With the significant advantages of nanoparticles, intensive research have been focused on the synthesis of various ecofriendly biologically active compounds utilizing nanocatalysts in order to fulfill greener methodologies which can eliminate or minimize the utilization of toxic and hazardous chemicals [xxi,xxii]. The green synthesis provides remarkable advantages like cost effective methodology, environmentally benign, milder reaction conditions, simple methods and easy work up procedures [xxiii-xxv]. In this connection, the *Aloe vera* mediated silver nanoparticles have attained significant attention. *Aloe vera* is considered as the most commonly used medicinal plants owing to its notable biological activities. The extract obtained from *Aloe vera* plant can act as a stabilizing and a reducing agent in the formation of silver nanoparticles.

***Different Types of Nanoparticles***

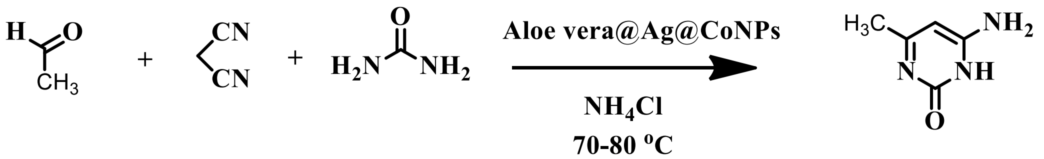
Based on literature survey, the distinctive reported types of nanoparticles (NPs) are photochromic polymer NPs, polymer coated magnetic NPs, inorganic NPs, AgNPs, CuNPs, AuNPs, SiNPs. Each of these NPs show diversified applications and they can be synthesized by various conventional as well as unconventional methods. Among them, silver is used most commonly as it is considered as innocuous, safe and antimicrobial agent which is used to inhibit the growth of microbes.

Antimicrobial properties of the nano-sized silver are better than that of silver ions. Because of the important applications, the synthesis of silver nanoparticles has attracted the attention of various research groups. [xxvi] The antibacterial activity of compound containing silver can be utilized in medicine in order to prevent the infections on the burn treatment, [xxvii,xxviii] to prevent bacteria colonization on catheters and to eliminate microorganisms on textile fabrics [xxix] as well as used as disinfectant in water treatment. Besides this, AgNPs are important as they have various applications in organic reactions, catalysis, synthesis of fine chemicals and organic intermediates [xxx]. Henceforth, the use of AgNPs in catalysis is advantageous as it avoids the use of ligands and easily separable catalyst for recyclability which makes the protocol economic.

Adopting the remarkable properties of silver nanoparticles of *Aloe vera,* the preparation of bioactive compounds using greener technology has been surveyed. In this connection, pyrimidine derivative, which is a heterocyclic compound containing two N atoms in the six membered ring, plays an important role in the field of chemistry. The pyrimidine and their derivatives play crucial role in medicinal chemistry like fungicidal, bactericidal, analgesic etc. Therefore, in present work, we have utilized a mild and cost effective conditions for synthesizing 6-amino-4-phenylpyrimidin-2(1H)-one.

***General Procedure for Synthesis of 6-amino-4-phenylpyrimidin-2(1H)-one***

A mixture of acetaldehyde (0.25 mmol), malanonitrile (0.12 mmol), urea (3 mmol), and 10 mg of *Aloe vera* AgCo NPs were taken in 5 ml of ethanol. The reaction was continuously stirred at 70-80 °C for 4 hours. The reaction was monitored with the help of TLC. After completing the reaction, it was cooled down and poured in the crushed ice to obtain the crude product. The product was filtered off and washed with the help of distilled water. It was recrystallized from ethanol for further spectral analysis. The $^1$HNMR spectrum of synthesized compound is represented in figure 2.




**Acetaldehyde (1)** **Malanonitrile (2)** **Urea (3)** **6-amino-4-phenylpyrimidin-2(1*H*)-one (4)**

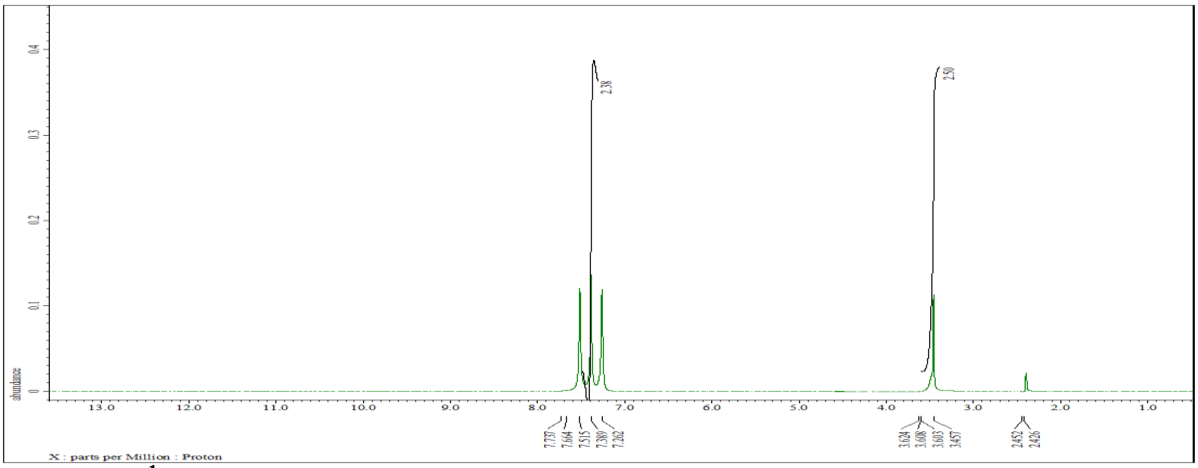



**Figure 2: $^{1}$H NMR spectra 6-aminopyrimidin-2(1H)-one 6-amino-4-phenylpyrimidin-2(1H)-one**

**Green Chemistry Metrics**

The green chemistry parameters highlight the aspects of a reaction relating to the twelve principles of green chemistry. Green chemistry metrics for the synthesis of 6-amino-4-phenylpyrimidin-2(1H)-one using *Aloe vera* @AgCoNPs were calculated. The details and calculations are provided in Table 1 and Table 3 respectively, which shows the closeness of the calculated values for the current methodology to the ideal values of the green chemistry parameters. Hence, it depicts the sustainability of present study.

**Table 1 Formula weight, mmol and amount of reactants and 6-amino-4-phenylpyrimidin-2(1H)-one**

| .Details | Acetaldehyde | Malanonitrile | Urea | Product |
|---|---|---|---|---|
| **Formula Weight** | 44 | 66.06 | 60 | 125.13 |
| **mmol** | 0.25 | 0.12 | 3 | 0.65 |
| **Amount (mg)** | 11 | 7.92 | 180 | 81.67 |

**Table 2: Calculation of green chemistry parameters for 6-amino-4-phenylpyrimidin-2(1H)-one**

| S.No. | Parameters | Formula | Characteristics | Ideal Value | Calculated value for compound |
|---|---|---|---|---|---|
| 1. | Environmental (E) factor | [Total mass of the raw materials – the total mass of the product] / mass of the product | E-factor gives the total amount of waste produces in the reaction. | 0 | [(11 + 7.92 + 180) - 125.13]/125.13 = 0.5 |

| | | | | | |
|---|---|---|---|---|---|
| 2. | Process mass intensity (PMI) | Σ (mass of all stoichiometric reactants)/[mass of the stoichiometric product] | PMI tells about reaction efficiency, stoichiometry, amount of solvent. | 1 | (11 + 7.92 + 180 ) / 125.13 = 1.5 |
| 3. | Reaction mass efficiency (RME %) | [mass of the product/ Σ(mass of all stoichiometric reactants)]x100 | RME gives information about atom economy, and stoichiometry. | 100% | [125.13/(11 + 7.92 + 180 )] x 100 = 62.93% |
| 4. | Carbon efficiency (CE %) | [Amount of carbon present in the product/ Total carbon present in the reactant] x 100 | CE represents the percentage of carbon present in the reactant which is left in the product. | 100% | [0.65 x 5 / (0.25 x 2 + 0.12 x 3 + 1x 3)] x 100 = 84.2% |

**Conclusion(s)**

In conclusion, a biologically active heterocyclic compound, 6-amino-4-phenylpyrimidin-2(1H)-one was successfully synthesized using the silver nanoparticles of *Aloe vera.* It was observed that the outcome was depending upon the efficiency of the synthetic route, the yield of the product and the purity of the synthesized compounds. The present protocol offered numerous advantages like easy work up of the desired product, reusability of the nanoparticles, the shorter reaction time, and cost effective. Moreover, from sustainability point of view, the green chemistry parameters such as Environment factor (E-factor), carbon efficiency (CE), reaction mass efficiency (RME) and atom economy (AE), were also calculated and reported. Therefore, the efficient and environment friendly silver nanoparticles can contribute to advancement in the nanotechnology. The continuous research will likely focus on optimizing synthetic routes to improve the scalability and cost effectiveness of the synthesized drugs.

**Acknowledgement**

Both the authors would like to acknowledge Department of Chemistry, Faculty of Science, Swami Vivekanand Subharti University, Meerut, UP for throughout support.

**References**

i. Basiago A. D.; Methods of defining ‘sustainability’; J. Sustain. Dev.; 1995, **3**(3), 109-119.
ii. Naidu R.; Biswas B.; Willett I. R.; Cribb J.; Singh B. K.; Nathanail C. P.; Aitken R. J.; Chemical pollution: A growing peril and potential catastrophic risk to humanity; Environ. Int.; 2021, **156**, 106616.

iii. Xu H.; Jia Y.; Sun Z.; Su J.; Liu Q.S.; Zhou Q.; Jiang, G; Environmental pollution, a hidden culprit for health issues; Eco-Environ. Health.; 2022, **1**(1), 31-45.
iv. Gavrilescu M.; Water, soil, and plants interactions in a threatened environment; Water.; 2021 , **13**(19), 2746.
v. Timmis K.; Ramos J. L.; The soil crisis: the need to treat as a global health problem and the pivotal role of microbes in prophylaxis and therapy; Microb. Biotechnol.; 2021, **14**(3), 769-797.
vi. Tong S.; Bambrick H.; Beggs P. J.; Chen L.; Hu Y.; Ma W.; Tan J.; Current and future threats to human health in the Anthropocene; Environ. Int,; 2022, **158**, 106892.
vii. Yu W.; Zhuang M.; Geng M.; Hu K.; Zhao Q.; Yan J.; Association between hydrometeorological conditions and infectious diarrhea in mainland China: a spatiotemporal modeling study; Environ. Res. Lett.; 2024, **19**(6), 064004.
viii. Taghavi M.; Bakhshi K.; Zarei A.; Hoseinzadeh E.; Gholizadeh, A; Soil pollution indices and health risk assessment of metal (loid) s in the agricultural soil of pistachio orchards; Sci. Rep.; 2024, **14**(1), 8971.
ix. Deng H.; Tu, Y.; Wang H.; Wang Z.; Li Y.; Chai L.; Lin Z.; Environmental behavior, human health effect, and pollution control of heavy metal (loid) s toward full life cycle processes; Eco-Environ Health.; 2022, **1**(4), 229-243.
x. Jiang G.; Preface to the special topic on environmental pollution and health risk.; Natl. Sci. Rev.; 2016, **3**(4), 409-409.
xi. Xu H.; Jia Y.; Sun Z; Su J.; Liu Q. S.; Zhou Q.; Jiang G; Corrigendum to “Environmental pollution, a hidden culprit for health issues; Eco-Environ. Health.; 2022, **1**(3), 198.
xii. Borah P.; Kumar M.; Devi P; Types of inorganic pollutants: metals/metalloids, acids, and organic forms; In Inorganic pollutants in water.; 2022, 17-31, Elsevier.
xiii. Rathi B. S.; Kumar P. S.; Vo D. V. N.; Critical review on hazardous pollutants in water environment: Occurrence, monitoring, fate, removal technologies and risk assessment; Sci Total Environ.; 2021, **797**, 149134.
xiv. Khan S.; Naushad M.; Govarthanan M.; Iqbal J.; Alfadul S. M.; Emerging contaminants of high concern for the environment: Current trends and future research; Environ. Res.; 2022, **207**, 112609.
xv. Li S.; Dong K.; Cai M.; Li X.; Chen X.; A plasmonic S-scheme Au/MIL-101 (Fe)/BiOBr photocatalyst for efficient synchronous decontamination of Cr (VI) and norfloxacin antibiotic; EScience.; 2024, **4**(2), 100208.
xvi. Pereira L. C.; de Souza A. O.; Bernardes M. F. F.; Pazin M.; Tasso M. J.; Pereira P. H.; Dorta D. J; A perspective on the potential risks of emerging contaminants to human and environmental health; Environ. Sci. Pollut. Res.; 2015, **22**, 13800-13823.
xvii. Puri M.; Gandhi K.; Kumar M. S.; Emerging environmental contaminants: A global perspective on policies and regulations; J. Environ. Manag.; 2023, **332**, 117344.

xviii. Nishanth Rao R.; Jena S.; Mukherjee M.; Maiti B.; Chanda K.; Green synthesis of biologically active heterocycles of medicinal importance: A review; Environ. Chem. Lett.; 2021, **19**, 3315-3358.
xix. Zuin V. G.; Eilks I.; Elschami M.; Kümmerer K.; Education in green chemistry and in sustainable chemistry: perspectives towards sustainability; Green Chemistry.; 2021, **23**(4), 1594-1608.

xx. Singh P.; Yadav, P.; Mishra A.; Awasthi, S. K.; Green and mechanochemical one-pot multicomponent synthesis of bioactive 2-amino-4 H-benzo [b] pyrans via highly efficient amine-functionalized SiO2@ Fe3O4 nanoparticles; ACS omega.; 2020, **5**(8), 4223-4232.

xxi. Riyadh S. M.; Khalil K. D.; Aljuhani, A.; Chitosan-MgO nanocomposite: One pot preparation and its utility as an ecofriendly biocatalyst in the synthesis of thiazoles and [1, 3, 4] thiadiazoles; Nanomaterials.; 2018, **8**(11), 928.

xxii. Behrouz S.; Rad M. N. S.; Piltan, M. A.; Ultrasound promoted rapid and green synthesis of thiiranes from epoxides in water catalyzed by chitosan-silica sulfate nano hybrid (CSSNH) as a green, novel and highly proficient heterogeneous nano catalyst, Ultrasonics Sonochemistry.; 2018, **40**, 517-526.

xxiii. Balciunaitiene A.; Viskelis P.; Viskelis J.; Streimikyte P.; Liaudanskas M.; Bartkiene E.; Lele, V; Green synthesis of silver nanoparticles using extract of Artemisia absinthium L.,; Humulus lupulus L. and Thymus vulgaris L., physico-chemical characterization, antimicrobial and antioxidant activity; Processes.; 2021, **9**(8), 1304.

xxiv. Naikoo G. A.; Mustaqeem M;, Hassan I. U.; Awan, T.; Arshad, F.; Salim, H.; Qurashi A.; Bioinspired and green synthesis of nanoparticles from plant extracts with antiviral and antimicrobial properties: A critical review; Journal of Saudi Chemical Society.; 2021, **25**(9), 101304..

xxv. Shivakumar M.; Nagashree K. L.; Yallappa S.; Manjappa S.; Manjunath K. S. Dharmaprakash M. S.; Biosynthesis of silver nanoparticles using pre-hydrolysis liquor of Eucalyptus wood and its effective antimicrobial activity, Enzyme and microbial technology.; 2017, **97**, 55-62.

xxvi. Bagheri A. R.; Aramesh N.; Hasnain, M. S.; Nayak A. K.; Varma R. S.; Greener fabrication of metal nanoparticles using plant materials: A review, Chemical Physics Impact.; 2023, **7**, 100255.

xxvii. Li H.; You Q.; Feng X.; Zheng C.; Zeng X.; Xu, H.; Effective treatment of Staphylococcus aureus infection with silver nanoparticles and silver ions; Journal of Drug Delivery Science and Technology.; 2023, **80**, 104165.

xxviii. May A.; Kopecki Z.; Carney B.; Cowin A; Antimicrobial silver dressings: a review of emerging issues for modern wound care; ANZ journal of surgery.; 2022, **92**(3), 379-384.

xxix. Liang D.; Liang W.; Zhang R.; Yang H.; Xie Q; Zhang Z; Liu J; Preparation of solid disinfectant for water treatment and mechanism of benzalkonium chloride immobilization on activated carbon; Journal of Environmental Chemical Engineering.; 2022, **10**(5), 108309.

xxx. Aravindakshan P.; Krishnamoorthy A.; Pal C.; Chang Y.Y.; Tan N. P. ; A Review on Silver and Zinc Oxide Nanoparticles as Antimicrobial Agents in Water Treatment Technologies; Nano Life.; 2022, **12**(03), 2230002..


Received on April 13, 2025.